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High-quality variational wave functions for small ^{4}He clusters

R. Guardiola and M. Portesi
Departamento de Física Atómica y Nuclear, Facultad de Física, 46.100-Burjassot, Spain

J. Navarro
IFIC (Centro Mixto CSIC Universidad de Valencia), Facultad de Física, 46.100-Burjassot, Spain

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We report a variational calculation of ground state energies and radii of $^4\mathrm{He}_N$ droplets ($3 \leq N \leq 40$), using the atom-atom interaction HFD-B(HE). The trial wave function has a simple structure, combining two- and three-body correlation functions coming from a translationally invariant configuration-interaction description, and Jastrow-type short-range correlations. The calculated ground state energies differ by around 2% from the diffusion Monte Carlo results.

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The research on liquid helium clusters has attracted a great interest both experimentally and theoretically [1,2]. This research allows for the analysis of the evolution of various physical properties for increasing size of the system, going from single atoms to the bulk. Helium clusters are expected to remain liquid under all conditions of formation, offering thus the possibility to study finite-size effects in the superfluid state [3]. Moreover, it has been suggested that Bose condensation could be detected by means of helium atom-cluster collisions [4]. The experimental research has faced the difficulties of size detecting the clusters. Recently, molecular beam diffraction from a transmission gratting [5] has proven to be successful to detect even the ^{4}He dimer [6], giving further impetus to the study of helium clusters.

As the atom-atom interaction is well-known and relatively simple, the solution of the Schrödinger equation has been obtained using several microscopic methods, mainly based on Monte Carlo techniques [7,8,9,10,11]. Variational Monte Carlo (VMC) calculations, using a Jastrow-like ansatz for the many-body wave function, are currently used for systems dominated by strong short-range interactions. The VMC wave functions are the input for diffusion Monte Carlo (DMC), Green function Monte Carlo or path integral techniques which provide essentially exact, within statistical errors, ground state energies of ^{4}He clusters at zero temperature. Conversely, these calculations constitute a useful benchmark to test other many-body methods.

In this work we present a new method of obtaining high-quality variational wave functions to describe small bosonic clusters. The basic idea is to write the trial wave function as the product of three terms, each of them with well defined roles. The first term is the familiar two-body Jastrow correlation factor, which controls the strong atom-atom repulsion at very short distances. The second term is related to a single-particle description of the cluster and is written as the product of N single particle wave functions referred to the center-of-mass coordinate; it provides the required confinement of the constituents and fixes basically the size of the droplet. Finally, the third term corresponds to a special version of the configuration interaction (CI) expansion describing two- and three-particle excitations, its role being to incorporate fine details to the wave function for medium and long ranges, as well as some collective effects. In summary, the trial wave functions we shall consider to describe the ground state of $^4\mathrm{He}_N$ clusters is

$$\Psi(\mathbf{R}) = \prod_{i<j} g(r_{ij}) \Phi(\mathbf{R}) \left(1 + \sum_{i<j} f_2(r_{ij}) + \sum_{i<j<k} f_3(r_{ij}, r_{ik}, r_{jk}) \right), \tag{1}$$

where $\mathbf{R}$ represents all single-particle coordinates. The two-particle function $g(r_{ij})$ is the two-body Jastrow correlation. We shall use the form

$$g(r) = \exp\left(-\frac{1}{2} \left(\frac{b}{r} \right)^{\nu} \right), \tag{2}$$

introduced by McMillan [12] many years ago for the description of the homogeneous liquid using a 12-6 Lennard-Jones interaction, with the value $\nu = 5$ as required by Kato's cusp condition. Many VMC calculations have shown that this form is also appropriate when dealing with interactions of the Aziz type. For instance, in Ref. [10] fixed values $b = 3$Å, $\nu = 5$ have been used for the interaction HFDHE2 [13], independently of the number of constituents in the cluster. It makes sense to keep the same values for all the clusters, because this pair correlation should be determined only by the two-body interaction potential. We have slightly modified these values, employing $b = 2.95$Åand $\nu = 5.2$ in our calculations with the interaction HFD-B(HE) [14]. Note that, contrarily to other studies, we are considering for the Jastrow term only the dominant part at very short-ranges.

The function $\Phi(\mathbf{R})$ is the product of N single-particle wave functions $\phi(\mathbf{r}_i - \mathbf{R}_{CM})$, referred to the center-of-mass of the system. If ϕ is a gaussian (in other words, the 1s state of a harmonic oscillator potential), it may be written as

$$\Phi(\mathbf{R}) = \prod_{i<j} \exp\biggl(- \frac{\alpha^2}{2N} r_{ij}^2 \biggr), \tag{3}$$

depending on a size parameter α. Because of its Jastrow-like form we may absorb it into the definition of the Jastrow correlation factor, and define

$$\Phi_J(\mathbf{R}) = \prod_{i<j} \exp\left(-\frac{1}{2}\left(\frac{b}{r_{ij}}\right)^{\nu} - \frac{\alpha^2}{2N} r_{ij}^2 \right) \tag{4}$$

Our contribution to the variational description of the clusters is the term within parentheses in Eq.(1), with the pair f_2 and triplet f_3 correlations, which we have called above configuration interaction and will be abridged as CI2 and CI3 respectively. In previous works [17] we have extensively applied the CI2 scheme to the description of light nuclear systems, with less singular interactions than the usual atom-atom potentials. The method is based on a linearized version of the coupled cluster method (CCM) [15] at the SUB(2) and SUB(3) truncation approximation levels, restricted to translationally invariant excitations up to three particles-three holes. The linearized version of the CCM has been shown to be equivalent to a special configuration interaction scheme [16], much more efficient than the usual CI methods when dealing with realistic interactions. With respect to CCM, the CI scheme loses the cluster property and the correct scaling with the number of particles, being unappropriate for extended systems. However it is much simpler, as far as non-linear terms of the CCM expansion are absent.

The present mixed J-CI scheme may be compared with the correlated basis functions (CBF) method as developed by Feenberg, Clark and Krotscheck [18] for extended systems, in which Jastrow correlations are combined with non-orthogonal perturbation theory. The key concept behind both CBF and J-CI methods is to apply a divide-and-conquer strategy to the determination of the correlated wave function. It is known that Jastrow correlations are very well suited to treat the effects of the (strongly repulsive) short-range part of the interaction, whereas a CI approach can effectively deal with medium- and long-range correlations. In our approach, we substitute the standard configuration-interaction component by our conceptually equivalent but significantly more effective translationally invariant CI scheme. Note that we are combining additive CI and multiplicative Jastrow correlations.

The CI correlation functions f_2 and f_3 could be determined by minimizing the ground state energy, resulting in a system of coupled integro-differential equations for f_2 and f_3. As a practical alternative we have expanded these functions in a set of gaussians:

$$1 + \sum_{i<j} f_2(r_{ij}) + \sum_{i<j<k} f_3(r_{ij}, r_{ik}, r_{jk}) =$$
$$\sum_{p\le q\le r=1}^{N_\beta} C_{p,q,r}\, \mathcal{S} \left\{ \sum_{i<j<k} \mathrm{e}^{-\beta_p r_{ij}^2} \mathrm{e}^{-\beta_q r_{ik}^2} \mathrm{e}^{-\beta_r r_{jk}^2} \right\}, \tag{5}$$

where $\mathcal{S}$ indicates symmetrization with respect to the particle labels. The gaussian expansion has proven to be a very accurate representation of the correlation functions when both negative and positive values of β are included, with the only restriction of having a square integrable wave function. Among the set of parameters $\{\beta_p\}$ we fix one of them, say β_1, to zero. In this way we cover the three possibilities contained in the ansatz wave function: restricting the three labels p, q, r to 1, we deal (up to a normalization constant) with the correlated state Φ_J; keeping only two of these labels equal to 1, amounts to put on top of that state the linear two-body correlations; finally the unrestricted choice corresponds to the complete ansatz. Calculations presented later on will be referred as J, J-CI2 and J-CI3 results, respectively.

A convenient short-hand notation for the gaussian expansion is the following:

$$\sum_\mu C_\mu F_\mu(\mathbf{R}) \tag{6}$$

where the subindex μ refers to the ordered set ($p \le q \le r$), and

$$F_\mu(\mathbf{R}) = \mathcal{S} \left\{ \sum_{i<j<k} \exp\left(-\beta_p r_{ij}^2 - \beta_q r_{ik}^2 - \beta_r r_{jk}^2\right) \right\} \tag{7}$$

The variational determination of the energy reduces to the solution of a generalized eigenvalue problem, which can be stated as follows:

$$\sum_{\mu_2} \left(\mathcal{K}_{\mu_1,\mu_2} + \mathcal{V}_{\mu_1,\mu_2}\right) C_{\mu_2} = E \sum_{\mu_2} \mathcal{N}_{\mu_1,\mu_2} C_{\mu_2} \tag{8}$$

The matrix elements of the norm and the potential energy are the integrals

$$\mathcal{N}_{\mu_1,\mu_2} = \int \mathrm{d}\mathbf{R} |\Phi_J(\mathbf{R})|^2 F_{\mu_1}^*(\mathbf{R}) F_{\mu_2}(\mathbf{R}) \tag{9}$$

and

$$\mathcal{V}_{\mu_1,\mu_2} = \int \mathrm{d}\mathbf{R} |\Phi_J(\mathbf{R})|^2 F_{\mu_1}^*(\mathbf{R}) \sum_{m<n} V(r_{mn}) F_{\mu_2}(\mathbf{R}) \tag{10}$$

where $V(r)$ is the two-body interaction potential. For the matrix elements of the kinetic energy operator we choose to write them as

$$\mathcal{K}_{\mu_1,\mu_2} = \int \mathrm{d}\mathbf{R} |\Phi_J(\mathbf{R})|^2 F_{\mu_1}^*(\mathbf{R})$$
$$\frac{1}{\Phi_J(\mathbf{R})} \biggl(- \frac{\hbar^2}{2m} \sum_n \Delta_n \biggr) F_{\mu_2}(\mathbf{R}) \Phi_J(\mathbf{R}) \tag{11}$$

since we shall use the positive definite function $|\Phi_J(\mathbf{R})|^2$ as the guide of a Metropolis random walk [19]. Note that no substraction of the center-of-mass contribution is necessary, as we are using a translationally invariant wave function. The number of unkown amplitudes C_μ is $\binom{N_\beta+2}{3}$. As mentioned above, the J and J-CI2 cases can be extracted easily from the general wave function: indeed, they correspond to the first $d \times d$ block of the matrices and the first d amplitudes, with $d = 1$ and $d = N_\beta$, respectively.

The last point to be discussed is the selection of the set of parameters $\{\beta_p\}$. Our previous experience with nuclear systems indicates that this selection is not very critical, as far as a sufficiently large interval of length ranges $(1/\sqrt{\beta}_p)$ is included. In the calculations presented below we have used the set $\{\beta_p/\alpha^2\} = \{0, -0.05, 0.5, 1, 4\}$. Large values of β_p should not be used, to avoid competition with the Jastrow factor.

The computational algorithm consists in carrying out a random walk guided by $|\Phi_J(\mathbf{R})|^2$ as the probability distribution function to evaluate the norm, potential and kinetic matrices as given in eqs.(9-11). The only adjustable parameter to be determined by minimization is α, since the amplitudes C_μ are self-adjustable. A final warning is in order. It is well known that calculations involving the solution of a generalized eigenvalue problem like eq.(8) are prone to numerical instabilities, because the over-complete basis giving rise to the overlap matrix $\mathcal{N}$ may have a determinant close to zero. In our case, the Monte Carlo evaluation of the overlap matrix (9) results always in a positive matrix, and the possible numerical instabilities are related only to numerical rounding errors.

In Table I are collected our results for binding energies and unit radii, defined as $r_0 = \sqrt{5/3\langle r^2\rangle}/N^{1/3}$, where $\langle r^2\rangle$ is the square mean radius. Columns labelled J, J-CI2 and J-CI3 correspond to the sequence of trial wave functions previously explained. Columns labelled VMC and DMC display the results obtained by other authors using the same interaction.

Our lowest order approximation (J) should be compared with column VMC. It can be seen that our crude choice for the two-body Jastrow correlation (2) produces less binding than the quoted VMC results. The reason of these differences is quite clear: once the parameters b and ν have been fixed, there remains a single variational parameter (α) in Φ_J. In contrast, the referred VMC calculations use more elaborate forms for the trial wave function, including three-body correlation functions in some cases, and containing from 5 to 10 parameters. Note however, that these differences decrease when N increases.

The inclusion of the CI correlation function f_2 changes substantially the results. It can be seen that figures in columns VMC and J-CI2 are basically the same, within statistical errors, except for the cluster with $N = 40$. The J-CI2 values have been obtained by minimizing the energy with respect to α and the set of five amplitudes describing f_2. The resulting values of α are given in Table I. In some cases we have also performed calculations including up to nine gaussians. It turns out that the binding energy does not change significantly, in spite of a considerably increase of the computing time.

We finally refer to our best variational results, namely J-CI3. There are no adjustable parameters in J-CI3, because we took the value of α which minimizes the J-CI2 energy and the same set of five β exponents, the C_μ amplitudes being determined by solving the generalized eigenvalue problem. It can be seen in Table I that the ground state energies provided by the J-CI3 scheme are above DMC ones by about 2%, except at the extremes of the table. For $N = 3$ both J-CI3 and DMC energies agree within statistical errors, and for $N = 20$ and 40 the differences are at the level of 4%. In any case, the J-CI3 description always shows a large improvement with respect to the more elaborate VMC calculations displayed in Table I. Moreover, the values obtained for the unit radius are very close to the values given by DMC calculations.

It is interesting to show the sensitivity to the value of the size parameter α of the three levels of approximation. As a typical example, in Figure 1 are shown our results for the cluster with $N = 8$. For completeness this figure includes also two horizontal dotted lines, which represent the optimal VMC and DMC energies, and which are not related in any form to our parameter α. One observes that even if there is a strong dependence of J energies with α, this dependence almost disappears when f_2 and f_3 correlations are included. The flatness of J-CI2 and J-CI3 energies is an indication of the completeness of the basis used to describe these correlations.

In conclusion, we have presented in this paper a variational wave function for ^{4}He clusters. A simple Jastrow function of McMillan type is sufficient to screen the strong short-range atom-atom repulsion, whereas the remaining medium- and long-range correlations seem to be adequately described by linear CI correlation functions. These functions are authomatically determined once given the size parameter α, which is the only adjustable parameter. We have shown that these variational wave functions produce high-quality results for small clusters. The method is likely applicable to other bosonic systems.

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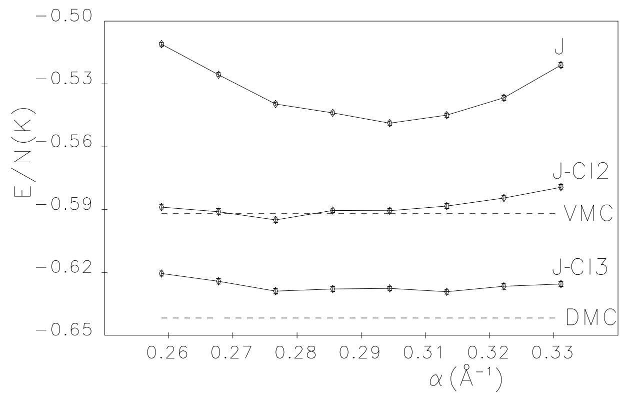

FIG. 1. Ground state energy per particle of cluster $^4He_8$, as a function of the inverse length parameter α, for the sequence of trial wave functions J, J-CI2 and J-CI3. VMC and DMC results are taken from Ref. [11].

TABLE I. Ground state energies per particle and unit radii of ^4He_N droplets, using the interaction HFD-B(HE). VMC and DMC energies are taken from [11] for $N \leq 10$, and [2] otherwise. DMC radii are taken from [9].

	E/N (K)						r_0 (Å)	
N	J	J-CI2	J-CI3	VMC	DMC	α(Å^{-1})	J-CI3	DMC
3	+.0136(4)	−.0373(8)	−.0430(10)	−.0385(3)	−.0436(2)	.18	5.4(2)	5.59
4	−.0835(7)	−.1326(13)	−.1398(15)	−.1333(10)	−.1443(2)	.22	4.11(11)	4.13
5	−.1984(8)	−.2502(14)	−.2616(13)	−.2506(3)	−.2670(3)	.25	3.66(7)	3.65
6	−.3187(11)	−.3678(12)	−.3868(11)	−.3676(2)	−.3950(2)	.27	3.42(6)	
7	−.4360(9)	−.4823(13)	−.5081(12)	−.4845(4)	−.5206(4)	.27	3.31(5)	3.22
8	−.5489(11)	−.5949(14)	−.6289(13)	−.5919(5)	−.6417(4)	.28	3.18(4)	
9	−.6531(10)	−.6995(13)	−.7392(12)	−.6924(5)	−.7563(6)	.28	3.11(3)	
10	−.7522(11)	−.7945(16)	−.8484(19)	−.7916(7)	−.8654(7)	.30	3.01(3)	
14	−1.0908(12)	−1.130(2)	−1.215(2)	−1.1290(7)	−1.2478(12)	.28	2.91(2)	2.83
20	−1.4743(16)	−1.5106(2)	−1.6336(15)	−1.510(2)	−1.688(2)	.30	2.727(14)	2.69
40	−2.218(3)	−2.273(3)	−2.4563(14)	−2.430(2)	−2.575(3)	.28	2.578(8)	